ACCESSION NUMBER: 108:21130 CASREACT Full-text
TITLE: Conformational analysis of organic carbonyl compounds.
Part 5. p-Methoxybenzoyl derivatives of benzo[b]furan, benzo[b]thiophene, and naphthalene
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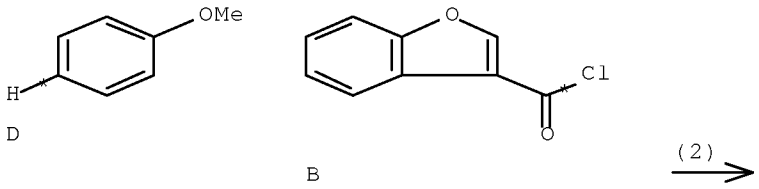
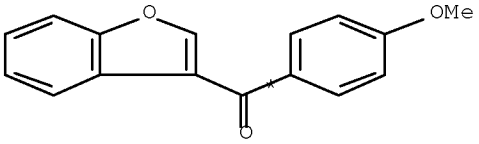
SOURCE: Journal of the Chemical Society, Perkin Transactions
2: Physical Organic Chemistry (1972-1999) (1987),
(3), 351-7
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The conformational anal. of 2- and 3-(p-methoxybenzoyl)benzo[b]furan and -benzo[b]thiophene and 1- and 2-(p-methoxybenzoyl)naphthalene was performed by the NMR lanthanide-induced shift method on 1H and 13C chemical shifts with Yb(fod)3. In the 2-substituted benzo[b]furan a chelate structure having the lanthanide atom bound to both carbonyl and furyl oxygens is formed, so the results do not represent useful information for the conformational properties of the mol. in solution For the 2-benzo[b]thiophene derivative the S,O-cis (Z) conformation was found to be more abundant in the equilibrium mixture of the two nearly planar conformers. In the corresponding 3-substituted heterocycles the predominant conformation is that of X,O-trans type with a similar degree of distortion from planarity in the two compds. In all these mols. the p-methoxyphenyl ring is twisted .apprx.30° from the carbonyl plane.

RX(2) OF 4 ...D + B ===> E

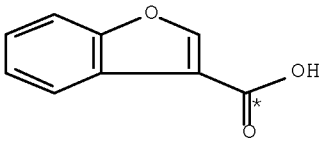




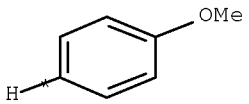
E
YIELD 44%

RX(2) RCT D 100-66-3, B 111964-21-7
RGT F 7446-70-0 AlCl3
PRO E 28222-80-2
SOL 75-15-0 CS2

RX(4) OF 4 COMPOSED OF RX(1), RX(2)
RX(4) A + D ===> E

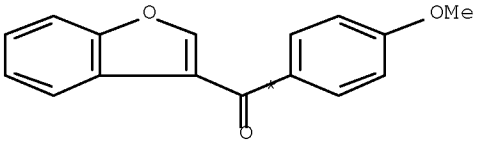


A



D

2
STEPS



E
YIELD 44%